

PREDICTION OF HYDROGEN CONSUMPTION FOR  
UPGRADING OF PYROLYSIS LIQUIDS<sup>1</sup>

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INTRODUCTION AND BACKGROUND

High performance aircraft require fuels with maximum heat of combustion per unit volume to achieve their maximum performance. A special class of hydrocarbon liquids can offer a relatively high energy density, fuel stability, high boiling point, and low viscosity. These fuels include bicyclic compounds composed of five- and six-ring structures such as decalin and biphenyl. Their heats of combustion range from 8800 to 9600 cal/ml versus 8000 cal/ml for JP-6 (Letort, 1962). On a volume basis such fuels would thus increase an aircraft's traveling range by 10-20%. Production of such fuels from petroleum (much of which is imported) derivatives appears to be relatively expensive. In contrast, coal liquids produced from low temperature pyrolysis or "mild gasification" may provide a rich source of aromatic bicyclics. These occur predominantly in the naphthalene or "heart-cut" of about 220-350°C boiling range (Hawk et al., 1965; Letort, 1962). Use of coal liquids however does require substantial upgrading to meet product specifications. Full boiling range liquids contain on the order of 60-75% aromatics, 1.6-10% oxygen, 0.5-3.0% sulfur, and 0.3-2.0% nitrogen (Gray et al., 1983; Hawk et al., 1965; Khan, 1986, 1987). Resulting jet fuels should meet specifications approximating those shown in Table 1.

Recent investigation at Naval Propulsion Center indicated that hydrogen content can serve as the decisive specification for aviation fuel quality (Moses et al., 1984; Masters et al., 1987). Investigators concentrated on combustion

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properties such as burning with minimal soot formation. They found that engines could operate satisfactorily on fuels with a hydrogen content below a reference of 13.8 wt%. Most engines could operate without adverse effects with fuels having a hydrogen content down to 13.3 wt%; and some, to 12.8 wt% of hydrogen. Likewise, Sullivan (1987) reported that fuels hydrotreated to meet combustion specifications should meet other specifications such as viscosity or freezing point.

A typical strategy for upgrading would include distillation of a heart-cut about 220-350°C. Severe hydroprocessing can be applied e.g., about 400°C and 2500 psig with a suitable nickel-containing catalyst. In some cases, it may be preferable to desulfurize first with a Co/Mo catalyst to improve the efficiency of the hydrogenation stage (Hawk et al., 1965). In addition it would be beneficial to hydrocrack 3-ring structures, phenanthrene, to 2-ring structure while limiting cracking of bicyclics.

Certain general observations can be made for the hydrogenation of a naphthalene heart-cut to low aromatics. First, the severe conditions noted above will essentially remove heterocyclic compounds from the products well before the <20 LV% aromatics specification is met. Therefore, there is no need to calculate incremental hydrogen consumption, but only a total consumption for given heteroatom content (Hawk et al., 1965; Eisen and Tice, 1977). Second, saturated and partially saturated bicyclics will dominate product composition. The degree of hydrogenation thus represents the extent of aromatic rings within a fairly stable, predictable molecular environment.

The objective of this study was to predict hydrogen consumption for conversion of a defined coal derived liquid to usable high density fuels. Literature on hydrogen consumption for upgrading coal derived liquids is extremely sparse. Many investigators do not determine hydrogen consumption in their studies. An excellent article published by Letort (1962) gave a clear picture of feed and product compositions and material balanced yields. The paper also reported hydrogen consumption for production of a high density jet fuel meeting JP-5 specification. Sullivan (1983) performed an extensive hydrotreating studies on upgrading a variety of coal derived liquids and determined the hydrogen consumption and jet fuel properties. Our analysis and subsequent predictions of hydrogen consumption are based on Letort's results with appropriate supporting data from Sullivan and others. This approach should be quite realistic for potential upgrading of bicyclic-rich coal derived heart-cuts.

## EXPERIMENTAL

The analysis presented in this study is based almost entirely on literature data, primarily reported by Letort. Letort (1962) performed a series of hydrogenation experiments on 230-310°C coal liquid distillate cut. The liquids were generated presumably in a commercial coal carbonization process. Hydrogenation experiments were performed in lab-pilot plant and commercial scale equipment. Calculations on hydrogen requirement were also performed based on the in-house data generated using a fixed-bed reactor. Detailed description of the reactor unit has been previously presented (Khan, 1987).

## RESULTS AND DISCUSSION

Upgrading mild gasification liquids into high quality fuels (e.g., high energy liquids) requires that the liquids be further treated to remove sulfur and nitrogen and to increase hydrogen content. This can be done by reacting the liquids with hydrogen gas. Ideally, the hydrogen required would be a product of the mild gasification process. While the amount of hydrogen required (approximately 2,000 SCF/bbl of liquids) is relatively low for the mild gasification process liquids, it is greater than the 10-20 volume percent (hydrogen) normally present in the mild gasification product gas. Typically, any additional required hydrogen is produced by gasifying the product char which adds process complexity; however, a preliminary experiment indicates that a calcium oxide bed can produce sufficient hydrogen by cracking methane and other hydrocarbon in the pyrolysis off-gas. In this experiment the gas products from coal pyrolyzed at 500°C were cracked over a bed of calcium oxide at 800°C. The product gas from the calcium oxide bed contained 50 percent hydrogen, which could be sufficient to totally upgrade the mild gasification liquids. Additionally, the hydrogen sulfide in the off-gas was greatly reduced by reaction with the calcium oxide. As an alternative, carbon monoxide and methane present in the product gas can be shifted and reformed to provide additional hydrogen.

Two approaches were used for hydrogen consumption calculation: (1) a simple approach using the H/C ratio of the feed and product streams; and (2) a more complex approach using molecular types in the feed.

In the simplified approach, hydrogen requirements for converting tars from different coals into usable liquids with H/C of 2. Table 2 presents the yields and analyses of tars from various coals from the fixed-bed reactor. Hydrogen consumption for upgrading the tars from fixed-bed reactor is compared to those from fluidized-bed reactor (Tyler, 1980; and Yeboah, 1980), from heated-grid reactor (Suuberg, 1979). Results on the hydrogen requirements (in gm of hydrogen needed to upgrade 100 g of raw pyrolysis liquids to a product with H/C of 2.0) from this comparison are plotted against the H/C in tars and coals as shown in Figure 1. It is noted from Figure 1 that an increase in hydrogen consumption occur with the decrease of H/C ratio of the raw tars. Figure 1 data also demonstrates that the liquids from the high heating rate processes such as fluidized bed and heated grid, have a smaller H/C ratio than those from a fixed bed reactor, which is a slow heating process.

Hydrogen consumption was also determined for a 180-280°C coal tar cut (Hawk et al., 1965) using this simplified approach. By material balance on the hydrogen content in the feed, product gas and product streams, hydrogen consumption of 5.16 SCF/100 lb of feed is estimated. This is in general consistent with the reported values.

In the second approach, the molecular structure and content for a 230-310°C coal tar distillate cut drawn from Letort's data were shown in Table 3. In this analysis the composition reported in Table 3 were taken as representative of the aromatic portion of a feedstock. For simplicity we are using this 100% aromatic-heteroatomic blend. In effect we are assuming that the saturated materials are carried through any given process as a diluent. Therefore one would use the methods presented here to calculate hydrogen consumption of the aromatic-heteroatomic portion and adjust results to reflect overall hydrogen

consumption on a "total barrel" basis. Table 4 shows expected reactions for hydrogenation and cracking of feedstock components. Note that phenanthrene is effectively converted to decalin.

In our analysis we have used the given feed, product compositions, yields, and reaction types outlined in Tables 3 and 4 to construct Tables 5a and 5b. This gives the distribution of products from each feed component upon upgrading. A number of modest assumptions were made regarding the material balancing of various ring structures. Table 6 summarizes hydrogen consumption calculations for the original base case from Letort (1962) leading to 19.82 LV% aromatic in the jet fuel cut.

In our analysis we have combined several pieces of information from Letort (1962). Letort hydrogenated a feed of the Table 3 composition to 10.2 LV% aromatics. He also reported a product component distribution. Using this product distribution as a guide we have estimated product distribution for a case of about 20 LV% product aromatics. (This aromatic content would be more in line with jet fuel specifications.) Essentially we assumed that the ring structure and degree of cracking between the two cases would be very similar with the main difference lying in a quantitative difference in the content of aromatic molecules. Working directly from the product distribution reported by Letort we doubled the content of aromatic products and accordingly decreased the amount of saturated product components. We then performed a lb mole balance analysis for the conversion of feed components to product components. This appears in Table 5a. We then determined the lb moles of  $H_2$  consumption to convert each lb mole of feed component to the respective product components. We present the hydrogen consumption for each product component in Table 5b.

In more detail, Table 5a presents an estimated product distribution for the hydrogenation of 100 lb of an aromatic feed described in Table 3 (Letort, 1962). Along each row are product components resulting from the hydrogenation of each feed component, listed on the left. For example, 0.328 lb moles of naphthalenes and alkyl naphthalenes enter as feed, of which 0.214 lb moles are converted to decalins; 0.0168 lb moles, to alkylindanes; and so forth. The total product components in each row equals the lb moles of feed, except where the feed molecule cracks into two molecules as noted by "x2" below the product amount.

From the product distribution estimates in Table 5a we calculated hydrogen consumption as presented in Table 5b. Values shown are estimated lb moles  $H_2$  consumed to convert feed components listed in the left hand column to the product components listed along each row.  $H_2$  consumption was estimated by multiplying the lb moles for each product component in Table 5a by the lb moles  $H_2$  required to convert the feed component (left hand column) to the product component in the same row. For example 0.328 lb moles naphthalenes/alkyl naphthalenes enter as feed and 0.214 lb moles are converted to decalins with 5 lb moles  $H_2$  required for each lb mole converted. Multiplying  $0.214 \times 5 = 1.07$  lb moles  $H_2$  consumed, listed under the column labeled "Decalins."

We also applied this estimation technique to Letort's data. We estimated a hydrogen consumption of 16.19 SCF/lb feed at 10.2 LV% product aromatics and a

product density (based on component densities) of 0.8696 g/cc. Letort (1962) reported 15.8 SCF/lb feed and 0.886 g/cc.

In order to estimate incremental hydrogen consumption we started with the initial case of 19.82 LV% aromatic in the product. The hydrogen consumption was then calculated for a case of 10.2 LV% product aromatics and the difference was calculated. Dividing by the change in aromatics gave an average incremental hydrogen consumption per LV% aromatics in the range of interest.

The average incremental hydrogen consumption, calculated is about 32 SCF/LV% aromatics/bbl in the 10-20 LV% range. This is comparable to the "rule of thumb" value (25 SCF/LV%aromatic/bbl) applied to petroleum distillate fractions. Note that once the fuel has been hydrogenated to about 20 LV% aromatics the hydrogen consumption for heteroatom removal approaches zero. Also note that in the original case much of the biphenyl cracks to a light cut (B.pt.<150°C) or gas. This is undesirable due to hydrogen consumption and destruction of a fuel component. The saturated dicyclohexyl has a heating value/ml about 12% higher than that for JP-6 (Letort, 1962).

It is very likely that satisfactory hydrogenation can be achieved with much less cracking. Hawk et al. (1965) hydrogenated comparable liquids with only 1.7 wt% loss to gases versus about 10% by Letort (1962). Sullivan (1983) reported losses to C<sub>4</sub> of less than 0.5%. Thus an optimum process should promote cracking of 3- to 2-ring species but suppress as much as possible the cracking of biphenyl. The benefits are threefold: (1) hydrogen consumption is lower than the other cases, (2) aromatics are lower, at 16.8 LV%, and (3) fuel cut yield is higher, at about 100 lb versus 85.5 lb for the two previous cases that exhibited the relatively large extent of cracking consistent with Letort's observation. Hydrogen consumption for three cases was considered by Letort, representing hydrogen consumption for a 100% aromatics feed to low product aromatics concentration of 10-20 LV%. On a barrel basis this would amount to about 5,000 SCF/bbl, a very high value. Sullivan (1983) gave more representative values, i.e. from 700-2,550 SCF/bbl, for a number of coal liquids hydrogenated to 20 LV% aromatics.

One should recognize that hydrogenation to about 20 LV% aromatics and consequently about 0 LV% heteroatoms is literally a given requirement. Further hydrogenation would be used to meet the remaining specifications, e.g., smoke point. Excessive hydrogenation must be minimized to conserve hydrogen and because hydrogenation generally reduces density.

The relationship between aromatic saturation and liquid properties is an interesting topic. Letort (1962) reported that his fuels ranged from 0-11 wt% aromatics and met freezing point and viscosity specifications for JP-5. Results from Eisen and Tice (1977) who used syncrudes from Utah and west Kentucky coals reveal the impact of percent aromatics on properties such as freezing, flash, and smoke points.

Comparing the data for each coal in the two aromatics ranges shows little change in physical properties below 25 LV% aromatics. Only smoke point and density change modestly. What this shows is that hydrogenation alone can be used to meet aromatics LV% and smoke point specifications. However, once aromatics have been reduced to about 20 LV%, properties such as flash or

freezing point will depend on more subtle characteristics of the mixture of molecular structures.

#### SUMMARY AND CONCLUSIONS

Based on a review of literature it appears that specific information on hydrogen consumption appears to be limited for upgrading of pyrolysis liquids. The appropriate tar fraction for upgrading to jet fuel is the 220-350°C cut which is composed of mainly aromatics with 2-ring structures with a minor amount of phenanthrene.

To achieve about 20 LV% product aromatics results in almost total heteroatom removal during the hydrogenation of aromatics.

For a 100% aromatic feed stream hydrogen consumption will be approximately 15.33/lb feed to yield 20 LV% product aromatics. However, typical values for actual coal liquids will range from 70-2,500 SCF/bbl. Suppression of cracking, perhaps through catalyst choice, could potentially reduce hydrogen consumption by 10-20% and improve product yields.

Incremental hydrogen consumption is about 30-32 SCF/bbl/LV% aromatics in the 10-20 LV% product aromatics range.

Additional aromatic saturation in the 10-20 LV% product aromatic range affects transport properties little, but does modestly affect smoke point and density.

Excessive hydrogenation must be avoided through choice of process conditions and catalysts because it wastes hydrogen and decreases density. Hydrogen content (12.8-13.3 wt%) may serve as the decisive specification for jet fuel quality.

It is important to crack phenanthrene to meet product specifications, e.g., viscosity, but biphenyl cracking should be suppressed. This conserves hydrogen and increases product yields with the saturated bicyclohexyl form, a high density fuel component.

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Table 1  
JP-5 Specifications  
(Risen and Tice, 1977)

Distillation, °F:		
10%.....	400	max
E.P.....	550	max
Gravity, °API.....	36-48	
Freezing Point, °F.....	-51	max
Aromatics, Vol.%.....	25	
Smoke Point, mm.....	19.0	min
Flash Point, °F.....	140	min
Viscosity, cSt -30°F.....	16.5	max

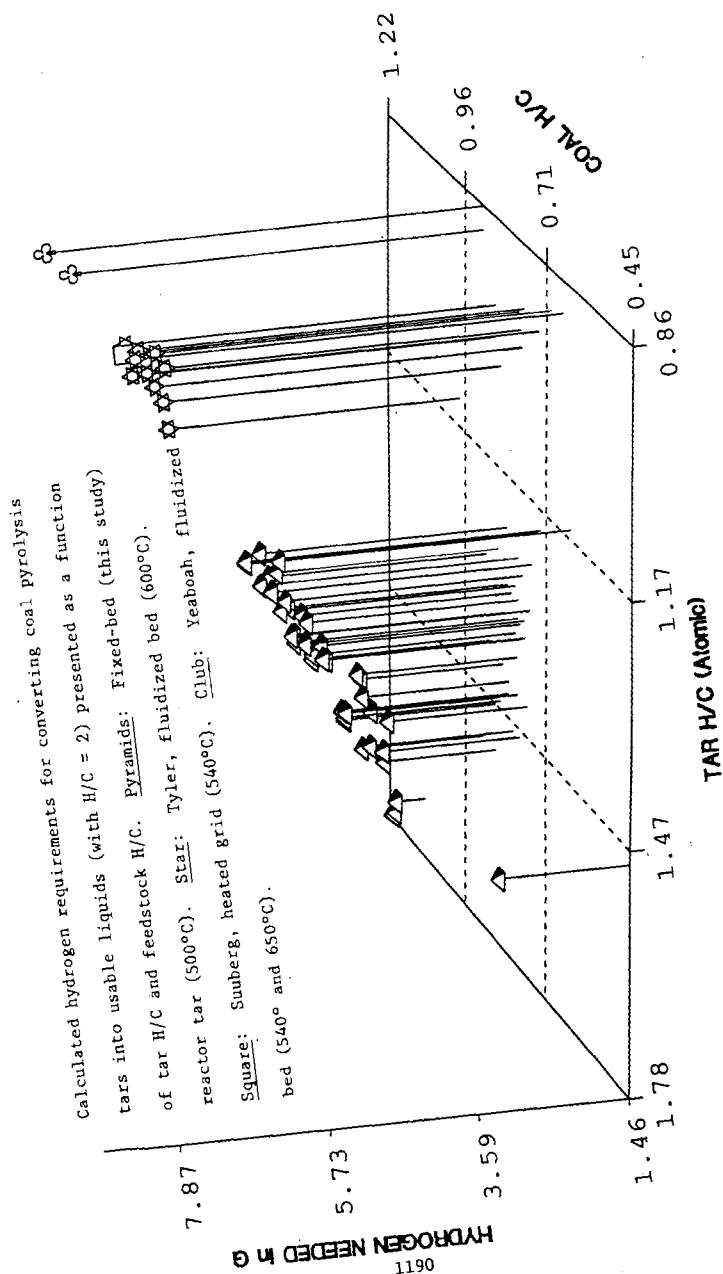


FIGURE 1





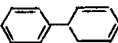






TABLE 2  
Yield and Analyses of Liquids Generated from Various Coal  
in the Fixed-Bed Reactor

OBS	Sample	Rank	Tar*	Gas (L)	Char*	Tar H	Tar C	H/C
1	PSOC 123	hvAb	14.8	6.04	75.2	10.19	84.89	1.44
2	PSOC 181	Sub A	13.8	7.90	81.9	9.36	83.01	1.35
3	PSOC 267	hvA	14.3	7.02	75.4	8.90	85.09	1.26
4	PSOC 275	hvAb	12.6	5.58	73.6	9.58	82.38	1.40
5	PSOC 296	hvAb	15.4	6.34	76.7	9.38	83.89	1.34
6	PSOC 306	hvAb	10.3	5.88	78.1	8.66	80.32	1.29
7	PSOC 355	hvAb	12.2	7.78	75.8	8.81	81.12	1.30
8	PSOC 375	hvAb	15.2	7.04	75.3	8.66	79.37	1.31
9	PSOC 1109	hvCb	25.0	9.29	56.6	11.66	78.70	1.78
10	PSOC 1313	mvb	5.5	6.02	84.7	8.59	85.91	1.20
11	PSOC 1323	hvBb	14.9	9.30	71.5	8.59	73.10	1.41
12	PSOC 1443	Sub C	10.5	9.80	66.6	10.33	80.93	1.53
13	PSOC 1445	hvC	14.1	9.80	69.5	10.78	84.51	1.53
14	PSOC 1448	hvAb	15.7	7.10	76.5	10.41	84.93	1.47
15	PSOC 1449	hvAb	23.6	7.12	62.3	11.06	78.04	1.70
16	PSOC 1451	hvA	14.1	3.10	80.5	8.70	82.01	1.27
17	PSOC 1469	hvAb	8.4	6.48	83.0	9.07	84.01	1.30
18	PSOC 1470	hvAb	9.2	3.82	76.8	8.22	80.08	1.23
19	PSOC 1471	hvAb	16.1	7.00	74.7	8.69	79.66	1.31
20	PSOC 1472	hvAb	14.8	8.06	76.2	9.37	86.03	1.31
21	PSOC 1473	hvAb	18.8	5.78	70.4	9.52	85.75	1.33
22	PSOC 1475	hvAb	15.8	7.84	75.1	10.08	84.58	1.43
23	PSOC 1481	hvAb	15.3	6.54	73.1	8.91	74.68	1.43
24	PSOC 1492	hvCb	13.7	7.90	70.5	8.60	74.67	1.38
25	PSOC 1499	hvAb	15.4	8.34	69.6	10.32	83.56	1.48
26	PSOC 1502	hvCb	12.7	8.40	69.9	10.01	81.07	1.48
27	PSOC 1504	hvAb	14.9	7.68	72.4	10.33	84.82	1.46
28	PSOC 1508	lv	3.2	5.50	91.0	--	--	--
29	PSOC 1516	lv	6.9	5.50	95.2	7.74	80.53	1.15
30	PSOC 1517	hvAb	14.2	8.60	75.3	8.88	79.73	1.34
31	PSOC 1520	Sub C	7.9	8.42	53.8	9.75	78.57	1.49
32	PSOC 1523	hvAb	12.7	6.30	80.5	9.25	83.66	1.33
33	PSOC 1524	hvAb	11.9	7.20	78.1	9.17	81.75	1.35
34	Pitts No. 8	hvAb	17.7	7.00	75.3	9.10	80.70	1.35
35	Ill. No. 6	hvCb	14.0	7.60	76.7	9.05	76.22	1.42
36	Ohio No. 6	hvCb	12.9	5.60	71.7	8.32	78.52	1.27
37	Wellmore No. 8	hvAb	14.2	7.00	75.6	8.76	84.30	1.25
38	AMAX	hvAb	14.1	7.70	77.1	8.53	85.86	1.19
39	N.D. Lignite	lig	4.0	11.40	64.1	9.14	75.04	1.46
40	Miss. Lignite	lig	21.3	13.00	54.2	11.40	77.80	1.76

\* Tar and char yield in weight percent (dry-basis)

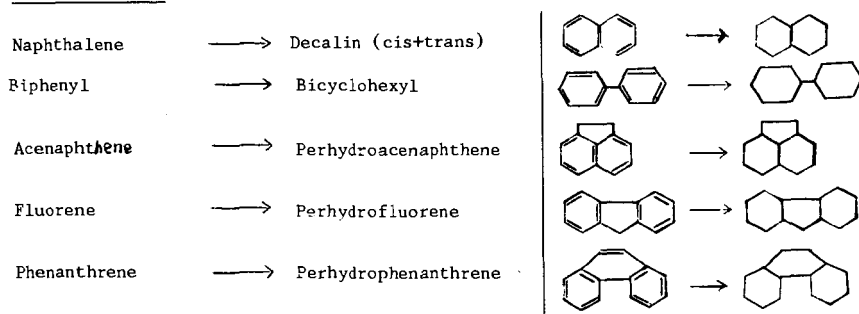
TABLE 3  
REPRESENTATIVE FEED COMPOSITION FOR COAL LIQUID AROMATICS

Formulas	Constituents	Weight %
	Light Constituents	1.1
	Naphthalene	10.3
	Quinolines	1.8 (0.2% Nitrogen)
	Alkyl Naphthalenes	38.7
	Biphenyl	5.4
	Acenaphthene	14.6
	Dibenzofuran	16.7 (1.6% Oxygen)
	Fluorene	6.9
	Phenanthrene	11
	Various Alkyl-biphenyls Alkyl-fluorenes	3.4
		<u>100.0</u>

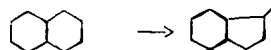
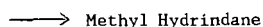
Tar fraction boiling between 230 and 310°C contains ring compounds in the quantities shown. Letort (1962).

TABLE 4  
TYPICAL REACTIONS FOR COAL LIQUID UPGRADING TO JET FUEL

RING SATURATION

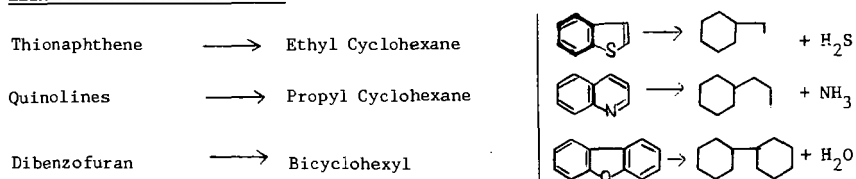


Isomerization  
Decalin



Ring saturation and isomerization reactions take these forms.

ELIMINATION OF HETERO ATOMS



CRACKING

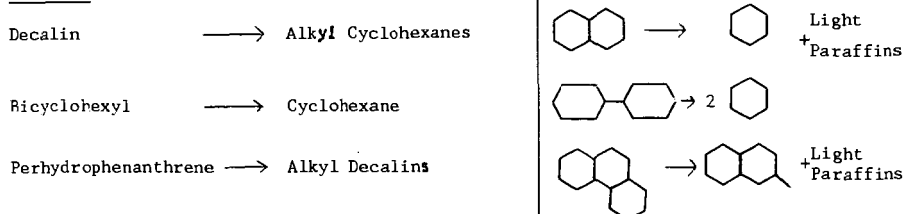


TABLE 5a

**ESTIMATED PRODUCT DISTRIBUTION FROM  
HYDROGENATION/CRACKING OF COAL TAR**

(values are feed, product lb moles on a 100 lb liquid feed basis)

19.8 LV% Product

Aromatics

Product Components

Feed Components

Feed	Alkyl-cyclohexanes	Decalins	Dicyclohexyl	Perhydro- acenaphthene	Perhydro- fluorene	Alkylbenzene	Alkylindanes	Tetralins	Cyclohexyl- benzene	Tetrahydro- acenaphthene	Hydrindanes	Phenanthrene
Light Constituents	.012	.008			.004							
Naphthalenes and Alkyl naphthalenes	.328	.214					.0168	.048			.05	
Quinolines	.014	.008				.006						
Biphenyl, Alkylbiphenyl, and Dibenzofuran	.144	.0005 x2	.026			.013 x2			.01			
Acenaphthene	.095	.041	.039				.0012	.0068		.003	.004	
Fluorene and Alkylfluorene	.051	.0033 x2			.0066		.003	.0032			.007	
Phenanthrene	.062	.0375					.003	.008			.009	.004
Product Totals		.3008	.026	.039	.0066	.036	.024	.066	.01	.003	.07	.004

presented here is an estimated product distribution for the hydrogenation of 100 lb of an aromatic feed described in Table 3 (Letort, 1962). Along each row, are product components resulting from the hydrogenation of the feed. The total product amount is 139 lb moles of naphthalenes and alkyl naphthalenes enters as feed, of which 0.214 lb moles are converted to decalins; 0.0168 lb moles, to alkylindanes; and so forth. The total product components in each row equals the lb moles of feed, except where the feed molecule cracks into two molecules as noted by "x2" below the product amount.

We derived the product distribution shown here for about 20 LV% aromatics from Letort's work in which he hydrogenated the given feed to 10.2 LV% product aromatics. For the estimate we doubled the product amount to 139 lb moles of product aromatics. The amount of saturated products, so as to material balance with the feed component in each row. We assumed that the extent of ring opening and other cracking reactions would remain little changed between the two cases.

TABLE 5b

**ESTIMATED HYDROGEN CONSUMPTION FOR PRODUCTION  
OF PRODUCT DISTRIBUTION IN TABLE 5a**

(Values are lb moles  $H_2$  consumed on a 100 lb feed basis)

19.8 LV% product

Aromatics

Product Components  $\rightarrow$

Feed Components  $\leftarrow$

	HDS, HDN, HDO	Alkyl- cyclohexanes	Decalins	Dicyclohexyl	Perhydro- acenaphthene	Perhydro- fluorene	Alkylbenzene	Alkylindanes	Tetralins	Cyclohexyl- benzene	Tetrahydro- acenaphthene	Hydrindanes	Perhydro- phenanthrene
Light Constituents		.024					0						
Naphthalene and Alkyl naphthalenes			1.07					.0326	.096			.35	
Quinolines	.042	.032					.006						
Biphenyl and Alkylbiphenyl Dibenzofuran	.2	.0035		.1296			.026			.03			
Acenaphthene			.082		.156			.0048	.0272		.006	.028	
Fluorene and Alkylfluorene		.184	.0664			.0396		.015	.016			.056	
Phenanthrene			.3375					.018	.048			.081	.028

Values shown are estimated lb moles  $H_2$  consumed to convert feed aromatics to the product components listed along each row. Product components are listed in Table 5a.  $H_2$  consumption was estimated by multiplying the lb moles of each product component in Table 5a by the lb moles  $H_2$  required to convert the feed component (left hand column) to the product component in the same row.

For example 0.328 lb moles naphthalenes/alkyl naphthalenes enter as feed and 0.214 lb moles are converted to decalines. The difference of 0.114 lb moles  $H_2$  required for each lb mole of naphthalenes/alkyl naphthalenes is listed under the column labeled "decalines".

TABLE 6  
SUMMARY OF HYDROGEN CONSUMPTION TO PRODUCE  
PRODUCT WITH 20 LV% AROMATICS  
(From feed described in Table 3)

Description of Hydrogen Consumption	H <sub>2</sub> Consumed
Aromatics Saturation	2.894 lb moles
Heteroatom Removal	0.242 lb moles
Production of Light Cut (<150°C)	0.365 lb moles
Production of Gases	<u>0.770 lb moles</u>
TOTAL:	4.271 lb moles H <sub>2</sub> /100 lb feed
	or 15.33 SCF/lb feed